

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
 Data File : VV021943.D
 Acq On : 25 Aug 2021 12:34
 Operator : SY/MD
 Sample : M3518-07ME
 Misc : 7.31g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AY9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M

Title : VOC Analysis

Signal : TIC: VV021943.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	113	rVB	119622	173948	13.07%	1.613%
2	2.076	313	322	333	rBV	269109	379480	28.52%	3.519%
3	2.490	444	451	469	rVB2	10381	19518	1.47%	0.181%
4	2.651	499	501	505	rVB3	398	224	0.02%	0.002%
5	2.732	521	526	527	rBV2	575	410	0.03%	0.004%
6	2.786	539	543	547	rBV2	315	270	0.02%	0.003%
7	2.960	594	597	598	rBV	411	197	0.01%	0.002%
8	3.008	609	612	614	rBV2	804	535	0.04%	0.005%
9	3.130	643	650	655	rBV3	290	284	0.02%	0.003%
10	3.243	683	685	690	rVB2	331	227	0.02%	0.002%
11	3.320	704	709	712	rVB2	226	176	0.01%	0.002%
12	3.339	712	715	717	rBV	311	190	0.01%	0.002%
13	3.670	813	818	822	rBV3	337	343	0.03%	0.003%
14	3.735	834	838	839	rBV2	435	265	0.02%	0.002%
15	3.789	851	855	858	rVB2	265	207	0.02%	0.002%
16	3.889	875	886	926	rBV	69571	262433	19.73%	2.434%
17	4.342	1010	1027	1059	rBV	189503	515431	38.74%	4.780%
18	4.561	1093	1095	1096	rBV	399	182	0.01%	0.002%
19	4.593	1103	1105	1107	rBV3	383	198	0.01%	0.002%
20	4.648	1116	1122	1123	rBV4	941	878	0.07%	0.008%
21	4.747	1150	1153	1156	rBV2	219	184	0.01%	0.002%
22	4.786	1162	1165	1170	rBV3	204	182	0.01%	0.002%
23	4.902	1197	1201	1206	rBV4	720	512	0.04%	0.005%
24	4.960	1215	1219	1222	rBV	284	188	0.01%	0.002%
25	5.037	1227	1243	1282	rBV2	531974	1330426	100.00%	12.337%
26	5.294	1318	1323	1325	rBV3	728	647	0.05%	0.006%
27	5.336	1325	1336	1353	rVV6	4494	13702	1.03%	0.127%
28	5.477	1378	1380	1382	rBV2	366	240	0.02%	0.002%
29	5.561	1402	1406	1409	rBV2	414	304	0.02%	0.003%
30	5.612	1409	1422	1449	rBV	435536	907807	68.23%	8.418%
31	5.831	1488	1490	1493	rBV2	401	268	0.02%	0.002%
32	5.902	1498	1512	1532	rBV2	32844	73010	5.49%	0.677%
33	6.069	1551	1564	1593	rVB	273481	597881	44.94%	5.544%
34	6.317	1636	1641	1642	rBV	407	289	0.02%	0.003%
35	6.464	1680	1687	1693	rBV4	692	1166	0.09%	0.011%
36	6.628	1733	1738	1740	rBV5	1051	1051	0.08%	0.010%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	6.728	1767	1769	1775	rVB2	781	542	0.04%	0.005%
38	6.760	1775	1779	1780	rBV	483	325	0.02%	0.003%
39	6.818	1793	1797	1799	rVB2	318	167	0.01%	0.002%
40	6.841	1802	1804	1810	rVB	408	273	0.02%	0.003%
41	6.985	1838	1849	1876	rBV	153234	302316	22.72%	2.803%
42	7.220	1915	1922	1926	rVB5	650	945	0.07%	0.009%
43	7.252	1928	1932	1933	rBV4	883	572	0.04%	0.005%
44	7.313	1940	1951	1970	rBV	637857	1126309	84.66%	10.445%
45	7.625	2037	2048	2075	rBV	102854	207182	15.57%	1.921%
46	7.773	2091	2094	2096	rBV3	418	336	0.03%	0.003%
47	7.799	2100	2102	2105	rVB4	726	252	0.02%	0.002%
48	7.821	2105	2109	2114	rVB4	655	829	0.06%	0.008%
49	7.847	2114	2117	2121	rBV2	423	357	0.03%	0.003%
50	7.931	2140	2143	2146	rBV	393	286	0.02%	0.003%
51	7.947	2146	2148	2152	rVV3	452	282	0.02%	0.003%
52	7.985	2155	2160	2162	rBV4	441	411	0.03%	0.004%
53	8.104	2184	2197	2228	rBV2	267457	625767	47.04%	5.803%
54	8.452	2303	2305	2307	rBV2	361	176	0.01%	0.002%
55	8.487	2314	2316	2320	rBV3	610	370	0.03%	0.003%
56	8.506	2320	2322	2324	rBV2	347	175	0.01%	0.002%
57	8.545	2332	2334	2337	rBV3	418	264	0.02%	0.002%
58	8.725	2387	2390	2392	rBV4	251	172	0.01%	0.002%
59	8.853	2418	2430	2453	rBV	652861	1133260	85.18%	10.509%
60	9.095	2503	2505	2509	rBV4	474	256	0.02%	0.002%
61	9.149	2518	2522	2529	rBV6	1803	2208	0.17%	0.020%
62	9.262	2553	2557	2561	rVB3	451	348	0.03%	0.003%
63	9.484	2619	2626	2627	rBV2	431	375	0.03%	0.003%
64	9.548	2643	2646	2654	rBV5	1678	2021	0.15%	0.019%
65	9.673	2680	2685	2690	rBV3	724	815	0.06%	0.008%
66	9.702	2690	2694	2698	rBV4	822	849	0.06%	0.008%
67	9.747	2705	2708	2712	rBV	244	191	0.01%	0.002%
68	9.943	2763	2769	2773	rBV2	678	908	0.07%	0.008%
69	9.982	2779	2781	2787	rVB	398	329	0.02%	0.003%
70	10.082	2809	2812	2814	rBV2	421	220	0.02%	0.002%
71	10.130	2818	2827	2837	rVB5	4782	8359	0.63%	0.078%
72	10.223	2844	2856	2877	rBV	383529	631468	47.46%	5.856%
73	10.448	2923	2926	2927	rBV2	611	324	0.02%	0.003%
74	10.458	2927	2929	2933	rVB3	789	431	0.03%	0.004%
75	10.513	2944	2946	2950	rVB	412	235	0.02%	0.002%
76	10.551	2951	2958	2959	rBV3	747	623	0.05%	0.006%

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 Title : VOC Analysis

77	10.667	2989	2994	3001	rVB4	832	898	0.07%	0.008%
78	10.699	3001	3004	3005	rBV	328	166	0.01%	0.002%
79	10.712	3005	3008	3013	rBV2	334	289	0.02%	0.003%
80	10.750	3013	3020	3022	rBV3	737	910	0.07%	0.008%
81	10.789	3029	3032	3035	rBV2	314	261	0.02%	0.002%
82	10.824	3039	3043	3048	rVV4	747	738	0.06%	0.007%
83	10.882	3056	3061	3064	rBV4	1052	1145	0.09%	0.011%
84	10.921	3067	3073	3084	rVB5	5624	8066	0.61%	0.075%
85	10.985	3091	3093	3097	rVB3	319	192	0.01%	0.002%
86	11.040	3102	3110	3114	rBV3	1115	1577	0.12%	0.015%
87	11.201	3156	3160	3164	rBV3	978	728	0.05%	0.007%
88	11.252	3164	3176	3195	rBV	817188	1267353	95.26%	11.753%
89	11.506	3253	3255	3258	rBV3	328	205	0.02%	0.002%
90	11.535	3261	3264	3267	rBV2	589	461	0.03%	0.004%
91	11.564	3271	3273	3274	rBV2	539	201	0.02%	0.002%
92	11.628	3281	3293	3314	rBV	743933	1159687	87.17%	10.754%
93	12.043	3418	3422	3427	rBV4	552	560	0.04%	0.005%
94	12.487	3558	3560	3563	rBV3	542	309	0.02%	0.003%
95	12.554	3579	3581	3584	rVB3	375	197	0.01%	0.002%
96	12.648	3606	3610	3617	rVB3	532	564	0.04%	0.005%
97	12.892	3678	3686	3693	rBV5	2081	2732	0.21%	0.025%
98	13.030	3726	3729	3730	rBV	444	269	0.02%	0.002%
99	13.194	3777	3780	3782	rBV2	393	268	0.02%	0.002%
100	13.271	3801	3804	3813	rVB4	823	1065	0.08%	0.010%

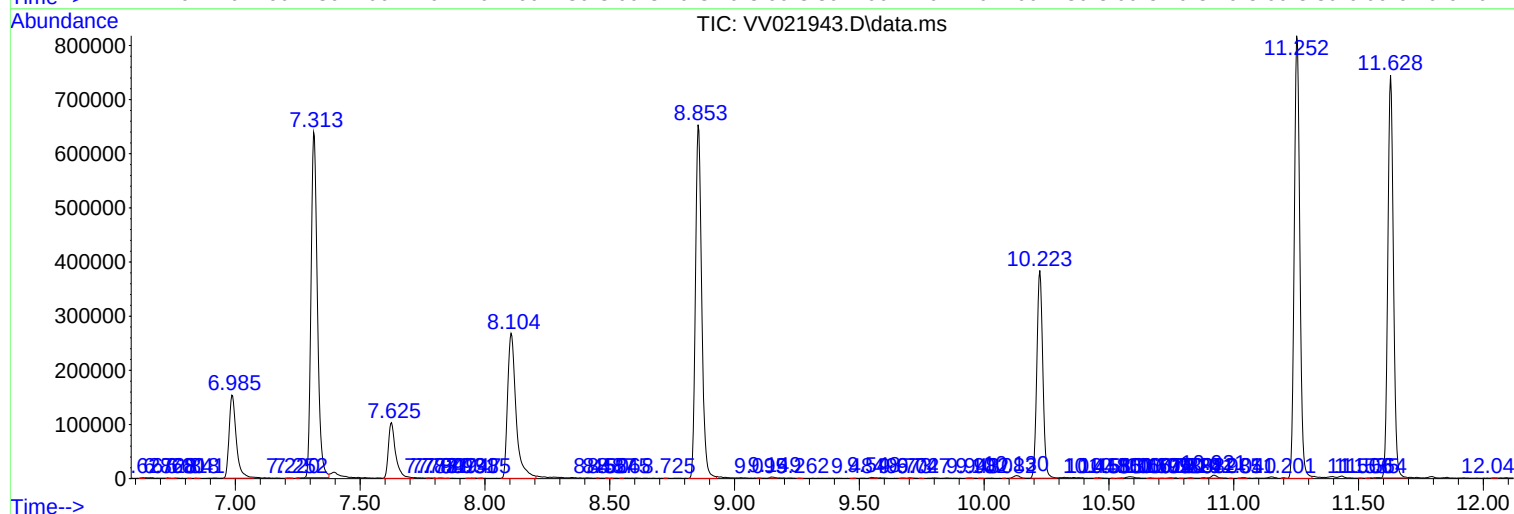
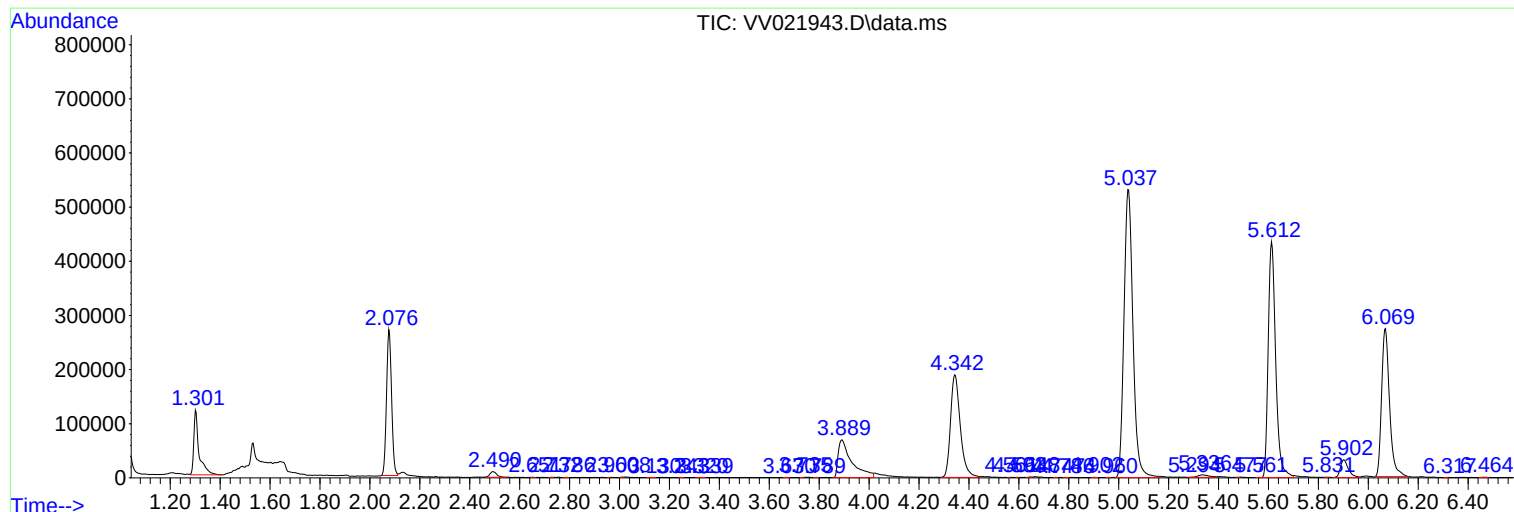
Sum of corrected areas: 10783622

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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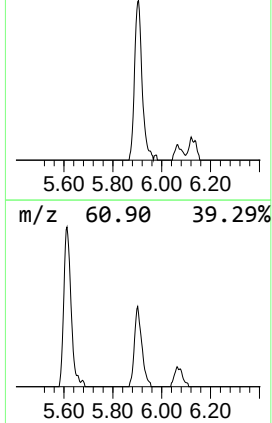
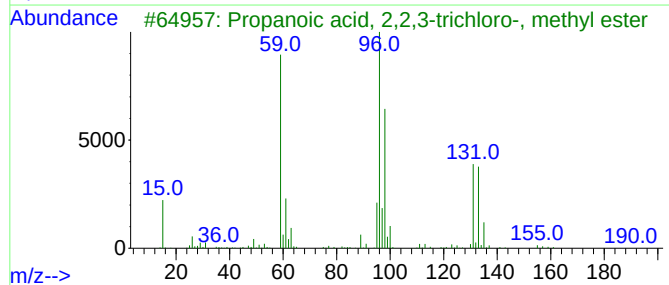
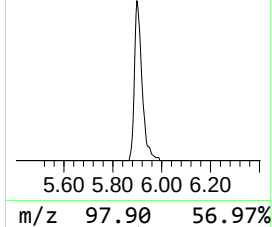
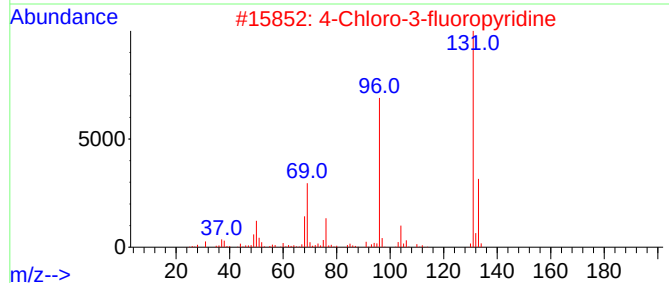
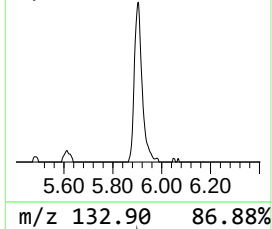
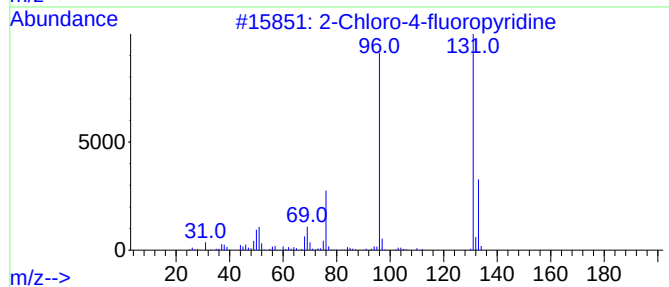
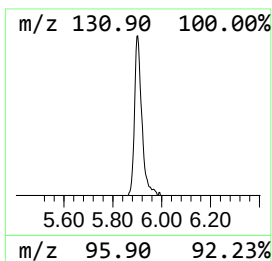
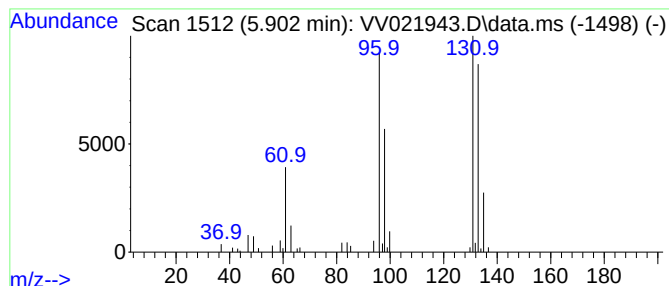
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	4.02 ug/L	73010	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
3			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
4			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	5.902	4.0	ug/L	73010	1	5.612	907807	50.0